

Monte-Carlo approach to particle-field interactions and the kinetics of the chiral phase transition

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Abstract. The kinetics of the chiral phase transition is studied within a linear quark-meson- σ model, using a Monte-Carlo approach to semiclassical particle-field dynamics. The meson fields are described on the mean-field level and quarks and antiquarks as ensembles of test particles. Collisions between quarks and antiquarks as well as the $q\bar{q}$ annihilation to σ mesons and the decay of σ mesons is treated, using the corresponding transition-matrix elements from the underlying quantum field theory, obeying strictly the rule of detailed balance and energy-momentum conservation. The approach allows to study fluctuations without making ad hoc assumptions concerning the statistical nature of the random process as necessary in Langevin-Fokker-Planck frameworks.

1. Introduction

One of the motivations for the study of ultrarelativistic heavy-ion collisions is to gain a detailed understanding of the phase diagram of strongly interacting matter [1]. At the largest energies as achieved at the Large Hadron Collider (LHC) and the Relativistic Heavy Ion Collider (RHIC) a hot and dense fireball is formed which can be described to a surprising accuracy as a nearly perfect fluid of strongly coupled quarks and gluons (QGP) undergoing a transition to a hot hadron-resonance gas. In these situations, where the net-baryon density or the baryon-chemical potential are small, lattice-QCD (lQCD) calculations indicate a crossover transition from confined to deconfined matter as well as from a phase where chiral symmetry is spontaneously broken to one where it is restored at a (common) transition temperature $T_c \simeq 160$ MeV [2].

At lower collision energies, as studied in the RHIC beam-energy scan (BES) program, at the CERN SPS, and the future FAIR and NICA experiments, the produced medium starts at lower temperatures and larger net-baryon densities. Since in this situation the application of lQCD is challenging due to the “sign problem” at finite μ_B , one relies on effective chiral models, which predict the existence of a first-order chiral-phase-transition line ending in a critical point of a second-order phase transition.

For theory the challenge is to provide possible observables for this phase structure in heavy-ion collisions, like the (“grand-canonical”) fluctuations of conserved charges like net-baryon number or electric charge. Not only the question, how to effectively model the phase transition (e.g., with the Nambu-Jona-Lasinio (NJL) or the (linear) σ model with extensions taking into account

gluonic degrees of freedom implementing Polyakov loops) arises but also, which of the features of the phase structure predicted for such models applying thermal quantum field theory (describing a medium in thermal and chemical equilibrium) like (critical) fluctuations of conserved charges survive for a rapidly expanding and cooling fireball as created in heavy-ion collisions.

To address the latter question, one relies on transport simulations to describe the off-equilibrium dynamics of the fireball. One approach is the use of ideal or viscous hydrodynamics to describe the bulk evolution of the fireball (assuming a state close to local thermal equilibrium), which successfully describes key phenomena of heavy-ion collisions, and adding the fluctuations by hand in a Langevin approach [3–5]. On the other hand this implies that the statistics of the random process has to be put in as an ad hoc assumption. Usually a Gaussian Markovian (“white noise”) is assumed, but the simulation of non-Markovian (“colored noise”) processes is feasible in principle [6].

On the other hand, one would like to study the implication of different transition scenarios (cross-over, 1st order, 2nd order) as realized in the various quantum-field theoretical models on the nature of the hopefully observable fluctuations [7–13] on the statistics of the probably observable fluctuations.

In this work we present a novel Monte-Carlo approach to address this challenging problem using the most simple quark-meson linear σ model [14]. The meson fields are treated on the mean-field level and the quarks and antiquarks are realized in terms of a test-particle ensemble. Here the challenge is to implement “discrete” local interaction processes like elastic collisions and reactions like the $q\bar{q}$ annihilation to a σ meson and the decay of σ mesons to a $q\bar{q}$ pair admitting not only kinetic but also chemical equilibration starting from an off-equilibrium situation, using the transition-probability matrix elements of the underlying quantum field theory.

2. Linear quark-meson σ model

To investigate the feasibility of a kinetic description of the off-equilibrium dynamics of the chiral phase transition the most simple two-flavor chiral model, based on the chiral group $SU(2)_L \times SU(2)_R$ is considered, using a flavor doublet of Dirac fields ψ , describing u and d quarks and antiquarks and a four-dimensional real-valued set of scalar fields $(\sigma, \vec{\pi})$ transforming under the $SO(4)$ representation of the chiral group [15]. The Lagrangian reads

$$\mathcal{L} = \bar{\psi}[i\not{\partial} - g(\sigma + i\gamma_5 \vec{p} \cdot \vec{\tau})]\psi + \frac{1}{2}(\partial_\mu \sigma \partial^\mu \sigma + \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi}) - U(\sigma, \vec{\pi}) \quad (1)$$

with the meson potential

$$U(\sigma, \vec{\pi}) = \frac{\lambda^2}{4}(\sigma^2 + \vec{\pi}^2 - \nu^2)^2 - f_\pi m_\pi^2 \sigma - U_0, \quad (2)$$

where $g \in [3.3, 5.5]$ denotes the Yukawa coupling between quarks and mesons, $\lambda^2 = 20$ the meson coupling constant (corresponding to a σ mass of $m_\sigma \simeq 600$ MeV), f_π the pion-decay constant, and $\nu^2 = f_\pi^2 - m_\pi^2/\lambda^2$. The potential (2) contains the explicit breaking of the chiral symmetry due to the finite current quark masses resulting in a non-zero pion mass, $m_\pi \simeq 138$ MeV, of the pseudo-Goldstone modes $\vec{\pi}$. The constituent quark masses are given by $m_q^2 = g^2 \sigma_0^2$.

The grand-canonical potential in mean-field approximation reads

$$\Omega(T, \mu) = U(\sigma, \vec{\pi}) + \Omega_{\bar{\psi}\psi} \quad (3)$$

with

$$\Omega_{\bar{\psi}\psi} = -d_n \int \frac{d^3 \vec{p}}{(2\pi)^3} [E + T \ln(1 + \exp(-\beta(E - \mu))) + T \ln(1 + \exp(-\beta(E + \mu)))], \quad (4)$$

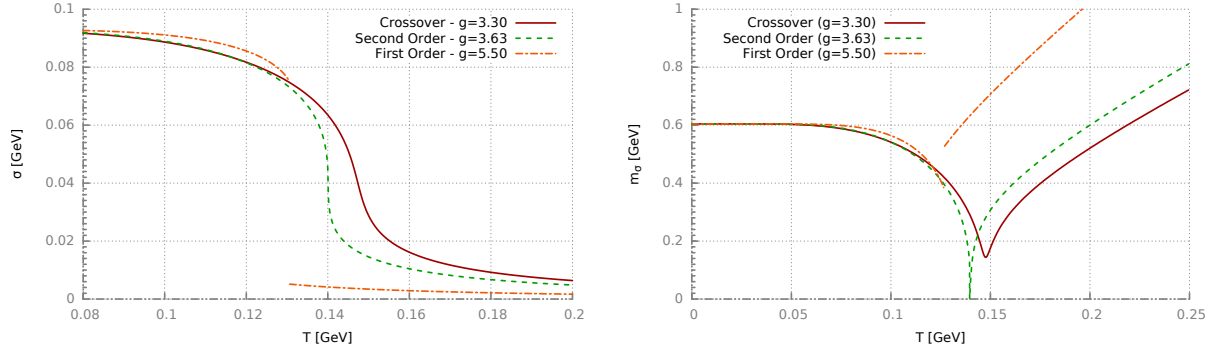


Figure 1. The phase diagram for the linear σ model in mean-field approximation at $\mu_B = 0$, $\langle \vec{\pi} \rangle = 0$. Left: the order parameter $\langle \sigma \rangle$ and the effective σ mass $m_\sigma = \partial^2 \Omega / \partial \sigma^2$.

where $E = \vec{p}^2 + g^2(\sigma^2 + \vec{\pi}^2)$ and the quark-degeneracy factor $d_n = 2N_f N_c = 12$. The mean fields have to be evaluated self-consistently from the equilibrium condition

$$\frac{\partial \Omega}{\partial \sigma} = \frac{\partial \Omega}{\partial \vec{\pi}} = 0. \quad (5)$$

In the following we restrict ourselves to vanishing pion mean fields. A nice feature of this model is that by varying the Yukawa coupling g , one finds different kinds of phase transition as illustrated in Fig. 1.

3. Semiclassical particle-field dynamics

The challenge in applying the above model to an off-equilibrium dynamical simulation of a system of particles (here quarks and antiquarks) and mean fields (representing the mesons) is that in order to reproduce the equilibrium-phase structure as depicted in 1 as the stationary limit, one has to ensure that both kinetic and chemical equilibration is possible through the introduction of the appropriate elastic collision terms for qq and $q\bar{q}$ scattering as well as quark-number changing processes such as $q\bar{q} \leftrightarrow \sigma$. In a full kinetic approach this is achieved by a set of coupled Boltzmann-Vlasov equations, which read in our case schematically (again restricting ourselves to the case of vanishing pion-mean fields)

$$\square \sigma + \lambda(\sigma^2 - \nu^2)\sigma - f_\pi m_\pi^2 + g \langle \bar{\psi} \psi \rangle = I(\sigma \leftrightarrow q\bar{q}), \quad (6)$$

$$\left[\partial_t + \frac{\vec{p}}{E_q} \cdot \vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}} E_\psi(t, \vec{x}, \vec{p}) \cdot \vec{\nabla}_{\vec{p}} \right] f_q(t, \vec{x}, \vec{p}) = C(\psi\psi \rightarrow \psi\psi, \sigma \leftrightarrow q\bar{q}). \quad (7)$$

Here, I and C denote collision integrals contributing to the meson-mean-field and quark-phase-space distribution functions respectively.

In the following a novel scheme to Monte-Carlo simulate such a system of kinetic equations is defined, where one describes the mesons solely with a mean field and the quarks and antiquarks in terms of test particles. While the elastic-collision term is realized in a straightforward way using the corresponding cross section from the underlying linear σ model, one has to find a way to realize the interactions $q\bar{q} \leftrightarrow \sigma$ in such a scheme, while still fulfilling energy-momentum conservation and the principle of detailed balance, which are the fundamental principles constraining the off-equilibrium dynamics and ensuring the proper (Maxwell-Boltzmann) equilibrium limit.

In our recently developed model (Dynamical Simulation of a Linear Sigma Model, DSLAM) this challenge is solved as follows: In order to properly simulate the collision terms on the right-hand sides of Eqs. (6) and (7) we define a space-time grid. In each time step at each spatial

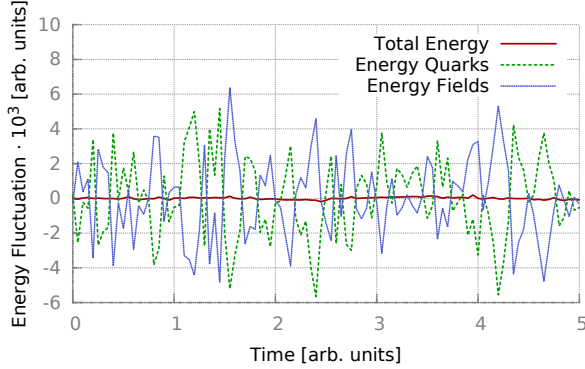


Figure 2. While the energies of the quarks and the meson field in the thermal-box simulation show anti-correlated thermal fluctuations of the order $\Delta E/E \sim 10^{-3}$ for the quarks and $\Delta E/E \sim 10^{-2}$ for the field the numerical fluctuations of the total energy amount to only $\Delta E/e \lesssim 5 \cdot 10^{-5}$.

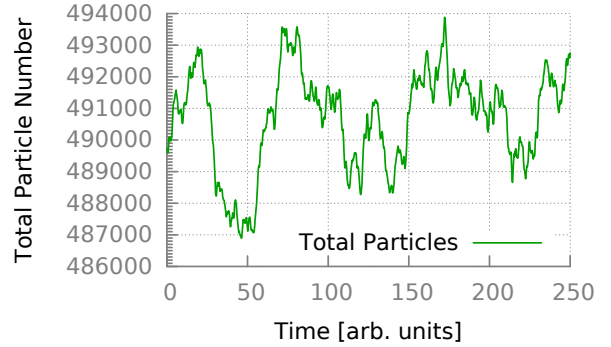


Figure 3. The total quark number in the thermal-box simulation shows fluctuations due to the dynamical pair-creation and annihilation processes, leading to an exchange of energy between the quarks and the mean field as shown in the left Fig. 2.

cell the cross section for the annihilation process $q\bar{q} \rightarrow \sigma$ is used to stochastically determine an energy-momentum transfer from the initial $q\bar{q}$ pair, located in the cell. This energy-momentum change is transferred to the σ mean field in terms of an appropriate relativistic Gaussian wave packet $\delta\sigma(t, \vec{x})$ (which simulates the gain term in I), and the $q\bar{q}$ pair is taken out of the test-particle ensemble (which simulates the corresponding loss term in C). To simulate also the appropriate decay process, $\sigma \rightarrow q\bar{q}$, we have to “particlize” the mean field locally in each spatial cell. This is done in the spirit of a course-graining procedure: First, the total energy-momentum content of the σ field within the cell in terms of the corresponding σ -field energy-momentum tensor is determined. Then one assumes a local thermal equilibrium phase-space distribution, equivalent to this energy-momentum tensor. In order to fulfill detailed balance, the temperature has to be the same as that for the corresponding procedure for the quarks and antiquarks. The temperature is related to the mean-field value which depends on the scalar quark-antiquark density. In this way a temperature can be determined. It is important to note that it is defined in the local rest frame of the heat bath and thus the σ -phase-space distribution is given by a Maxwell-Jüttner distribution $f_\sigma \propto \exp[-p_\mu u^\mu(t, \vec{x})/T]$, where u^μ is the four-velocity, given by the total field-four-momentum in the spacial cell under consideration, $u^\mu = p^\mu/E$. Now in each time-step within each spatial cell one can choose an ensemble of σ particles according to this local Maxwell-Jüttner distribution and using the corresponding $q\bar{q} \rightarrow \sigma$ decay rate to determine the gain term to C . The loss term for the mean-field equation in the collision term I is again achieved by taking the appropriate amount of energy and momentum out of the mean field in terms of a Gaussian wave packet.

In summary we have achieved a scheme which enables us to simulate the set of Boltzmann-Vlasov Eqs. (6) and (7) using test particles for the quarks and antiquarks and restricting the description of the mesons strictly to the mean-field level. The scheme by construction fulfills energy-momentum conservation through the Gaussian wave-packet description for the exchange of energy and momentum between the mean field and the test particles. At the same time also the principle of detailed balance is fulfilled, using the coarse-graining approach to locally map the field-energy-momentum distribution to a local-equilibrium Maxwell-Jüttner distribution to reinterpret the mean field as a meson phase-space distribution and using the leading-order transition rates (cross sections) of the underlying QFT linear σ model fulfilling the detailed-

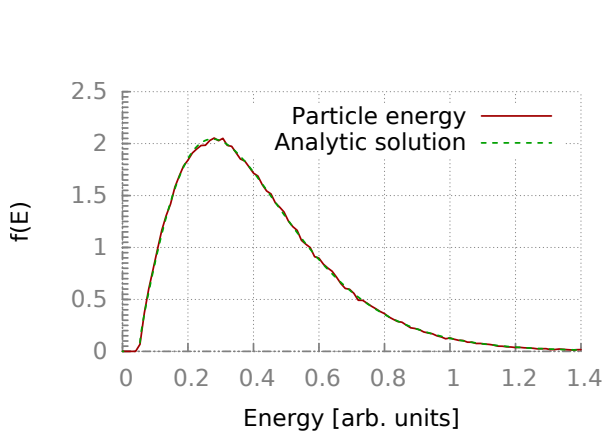


Figure 4. The distribution of the quarks' kinetic energy in a thermal-box calculation show an excellent agreement with the expected Maxwell-Boltzmann distribution.

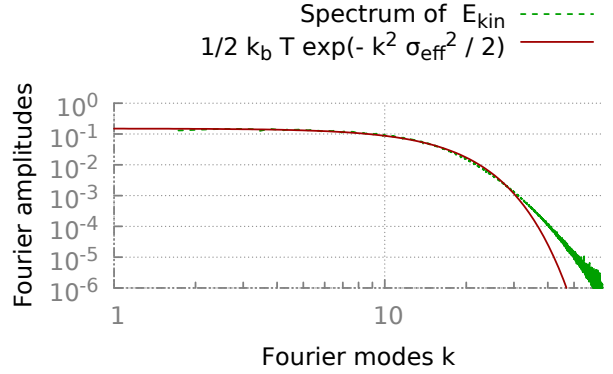


Figure 5. The distribution of the kinetic field energy to its Fourier modes. The classical “UV catastrophe”, i.e., the equipartition theorem associating an average energy of $k_B T/2$ for each Fourier mode, is avoided by the use of a finite finite width σ_{eff} of the Gaussian wave packets for the transfer of energy and momentum between particles and field.

balance principle.

4. Proof of principle: “Box” calculations

As a plausibility check of the simulation method the stability of an equilibrium situation has been tested in a finite cubic box with periodic boundary conditions [14]. The stability of the energy conservation is demonstrated in Fig. 2. While the kinetic energy of the quarks and the energy of the mean field show anti-correlated thermal fluctuations the total energy stays stable within the numerical accuracy of the simulation.

The annihilation and creation processes of quark-antiquark pairs lead to thermal fluctuations in the total particle number, as shown in Fig. 3.

The energy distribution of the quarks shows the expected Maxwell-Boltzmann distribution at the expected temperature, as demonstrated in Fig. 4. Also the spectral analysis of the mean field shows that the thermal equipartition theorem for the kinetic field energy is fulfilled at small wave numbers (long wavelengths), i.e., each mode contains an average energy of $k_B T/2$. On the other hand the “UV catastrophe” must be avoided due to the finite total-energy content within a finite box. Indeed, the energy-momentum transfer between particles and the field due to the pair-annihilation and -creation processes is not strictly “local” but occur within a finite volume whose scale is fixed by the finite width, σ , of the Gaussian wave packets used as field increments to keep care of the correct energy-momentum transfer in each process. Thus the large wave numbers (short wave lengths) are effectively cut off at a scale $k_{\text{cutoff}} = \sqrt{2}/\sigma$, as shown by plotting the corresponding Gaussian on top of the k -distribution of the kinetic field energy (Fig. 5).

The dynamical behavior of the field in our thermal-box simulation is illustrated in Fig. 6, showing the field distribution within the xy plane of the simulation. Starting the simulation with a uniform mean-field equilibrium value, after a short time some local blob-like disturbances have developed (left panel) due to quark-pair-annihilation processes, leading to the propagation of Gaussian wave packets on top of the still quite uniform average field value, as implemented by our concept of describing the exchange between field and particles in these processes. The right panel shows the fully developed equilibrium-thermal-field fluctuations in the long-time limit of

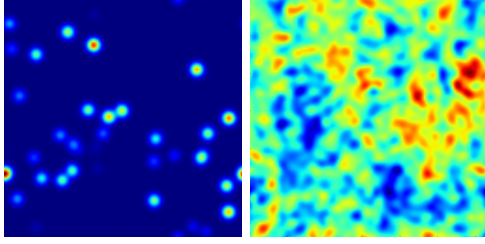


Figure 6. Starting with a uniform mean field, a short time after the start of the simulation the field is disturbed by some Gaussian wave packets due to quark-pair annihilation processes (left panel). In the long-time limit the full equilibrium-thermal-field fluctuations have developed.

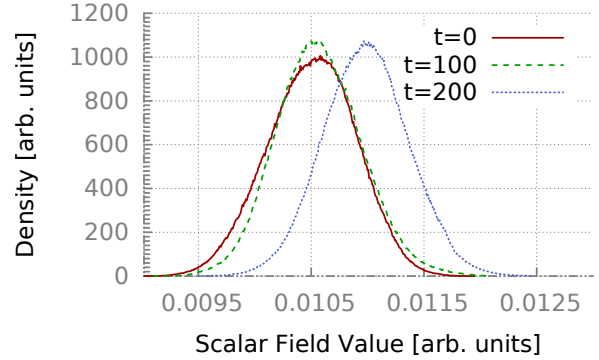


Figure 7. The field fluctuations are Gaussian distributed around an average value which can slowly drift with time due to the dynamical fluctuations of the field momentum.

the simulation. In this limit the field values are Gaussian distributed around a mean value (cf. Fig. 7), which is expected due to many random energy-momentum transfers between the field and particles. Thereby the average field value can slowly drift with time due to the thermal fluctuations of the field energy and momentum.

5. Conclusions and outlook

In this talk it was demonstrated that the dynamical description of the chiral phase transition in a simple quark-meson model is feasible with a novel Monte-Carlo-simulation technique for a corresponding coupled Boltzmann-transport equation for the meson mean-field and the quark and anti-quark phase-space distribution functions, implementing both elastic quark and anti-quark scattering as well as quark-antiquark-pair creation and annihilation processes, enabling both kinetic and chemical equilibration between particles and the mean field (mesons).

The simulation is set up in a way that both energy-momentum conservation and the principle of detailed balance are precisely realized (within the limits of achievable numerical accuracy). While the elastic quark-scattering processes are simulated with a straight-forward test-particle realization, the particle-field kinetics has demanded the development of a novel scheme.

The $q\bar{q} \rightarrow \sigma$ annihilation process is evaluated by the Monte-Carlo sampling according to the corresponding transition matrix elements from the underlying quantum-field theoretical interpretation of the linear σ model. The corresponding energy and momentum are precisely transferred to the σ -mean field in terms of an appropriate disturbance in form of a relativistic Gaussian wave packet. To obey the principle of detailed balance, also the inverse $\sigma \rightarrow q\bar{q}$ decay has to be simulated. To that purpose a coarse-graining procedure based on the local energy-momentum content of the field has been used for a “particlization” of the mean field in terms of a local Boltzmann-Jüttner equilibrium distribution, which in turn enables a Monte-Carlo sampling of the σ -meson decay according to the decay rate from the quantum-field theory picture of the model, which automatically implements detailed balance.

This scheme has now been applied to off-equilibrium situations as in a “thermal quench” in a box where the particles and fields are initialized with different temperatures and it was demonstrated that the distribution can describe a possible phase transition from the initial state to a late-time (equilibrium) state.

Last but not least also the case of “expanding fireballs”, mimicking the situation of the medium created in heavy-ion collisions, is under study.

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